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Relevance of liquid state to solid state properties*

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Abstract. We outline in this talk the beginning of a new programme to study physical properties of crystalline solids. It is based on considering the latter, a broken symmetry phase, in terms of the higher symmetry liquid phase. The solid is a calculable perturbation on the fluid. This is exactly opposite to the standard approach which relates mechanical properties to the behaviour of defects (mainly dislocations) etc., in an otherwise perfect crystalline solid. However, most other broken symmetry phases (*e.g.* ferromagnets) are discussed starting from a symmetric Hamiltonian or a free energy functional, and earlier work by one of the authors shows that the liquid-solid transition is well described, qualitatively and quantitatively, by this approach. On the other hand, defect theories of melting have a long record of nonsuccess. In the first part of the talk, the density wave theory of freezing will be outlined, and it will be shown how properties such as Debye Waller factor, entropy change of freezing etc. can be calculated with no or one free parameter. The problem of calculating shear elastic constants and dislocation core structures as well as energies in terms only of observable liquid state properties will be set up, and results presented. The method will be contrasted with zero temperature 'atomistic' models which obscure the essential dependence on structure and flounder in a mass of detail. The concluding part will describe further proposed applications, some suggestive experimental results extant in the literature, and some speculations.

Discussion

G Venkataraman: Is something like the Josephson effect possible in this case of change of phase associated with ballistic motion or diffusion?

T V Ramakrishnan: This is a hard question to answer.

V Balakrishnan: What stabilizes the system against other possible μ_G's? How does the system choose, say, between the fcc and bcc structures?

Ramakrishnan: We examine the stability of the fluid with respect to a *given* structure.

V Balakrishnan: What is it in the system that kills fluctuations with other wavevectors?

Ramakrishnan: The correlation function $S(q)$ is strongly peaked at a particular q. Thus the energy to excite this mode is far less than that for any other mode.

G Ananthakrishna: How does one measure the three-point correlation?

Ramakrishnan: This can be estimated either by computer simulation or by doing light scattering experiments on colloidal crystals.

G Srinivasan: Could one find the pressure dependence of the two-point correlation?

Ramakrishnan: This does not give the quantity required here.

* Only a summary is presented.

K R Rao: Is it necessary that the three-point correlation measurement be done in solid state?

Ramakrishnan: No. A "combination" scattering experiment has to be done in the liquid state for information in the short-range region.

K R Rao: What is the difficulty in predicting the melting temperature?

Ramakrishnan: The difficulty is that μ_G and C_G are dimensionless quantities.

S Ranganathan: Can your theory take into account the liquid-glass transition?

Ramakrishnan: No. We are very far from it.

D Dhar: How is the effective potential you use related to the effective potential used in cell theories of melting?

Ramakrishnan: The two are not related to each other.

S R Shenoy: Can one use your theory to handle a crystal with frozen-in defects?

Ramakrishnan: Perhaps one could, depending on how perfect these crystallites are and also on how rapidly the phase changes.

R Chidambaram: Where is the entropy of melting in this model?

Ramakrishnan: We calculate the entropy of melting from the known thermodynamic functions.

G Ananthakrishna: How do you describe dislocations and vacancies in your model?

Ramakrishnan: I don't know how to describe vacancies, but dislocations can be described in a manner similar to vortices in a superconductor.